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Covariance study of the LIUQE algorithm

Lab Report n°2

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Abstract

The new LIUQE algorithm computes a real-time reconstitution of the plasma in TCV, which gives interesting perspectives of tokamak control. Its computation relies on multiple linear regression. The study is introduced with theoretical features on regression in LIUQE algorithm and error propagation. Covariance and correlation matrices, as well as standard error values for parameters of regression are then computed on a TCV shot, allowing to study the effects of weights and the propagation of errors in the algorithm. The analysis of results focuses on improving the tuning of the algorithm: the optimal weights for plasma current and toroidal flux are determined, and redundant weighting is highlighted. The propagation of errors in the algorithm confirms also that a two basis function model is preferable to a three basis function model in the regression.

1 Introduction

1.1 Regression analysis

A few elements of notation for regression analysis are described in annexes.

1.1.1 The LIUQE regression

The equations of MHD can be used to describe the plasma equilibrium in the TCV. A few calculations [3] in cylindrical coordinates lead from these equations to the following result :

$$\Delta^* \psi = -2\pi\mu_0 r j_\phi \quad (1)$$

with the definitions of the operator and the current density:

$$\Delta^* = r \frac{\partial}{\partial r} \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \quad (2)$$

$$j_\phi = 2\pi \left(\frac{dp}{d\psi} + \frac{T}{\mu_0 r} \frac{dT}{d\psi} \right) \quad (3)$$

where p is the pressure. p and T are only functions of ψ . The combination of 2 and 3 gives the Grad-Shafranov equation at the core of the LIUQE algorithm:

$$\Delta^* \psi = -4\pi^2 \mu_0 r \left(rp' + \frac{TT'}{\mu_0 r} \right) \quad (4)$$

This equation is non-linear, and requires specific algorithmic methods.

1.1.2 Weighting the parameters

Matrix system for regression The values of the set of free parameters on the inner computational grid are stored in a rectangular matrix:

$$T_{yg} = r_y^{\nu_g} g_g(\psi(r_y, r_z)) \Delta r \Delta z \quad (5)$$

With this, the expected measurements can be written in matrix notation (cf [1], page 18, with the same notation):

$$\begin{array}{c} \text{measurements} \\ \left[\begin{array}{c} \psi_f \\ B_m \\ I_a \\ I_s \\ I_p \\ I_t \\ \Phi_t \end{array} \right] \end{array} = \mathbf{AdG} \cdot \begin{array}{c} \text{parameters} \\ \left[\begin{array}{c} J_a \\ J_s \\ a_g \\ \delta z \end{array} \right] \end{array} \quad (6)$$

$$\mathbf{AdG} = \begin{bmatrix} M_{fa} & M_{fs} & M_{fy} \cdot T_{yg} & \partial_{z_f} M_{fy} \cdot I_y \\ B_{ma} & B_{ms} & B_{my} \cdot T_{yg} & \partial_{z_m} B_{my} \cdot I_y \\ 1_a & 0 & 0 & 0 \\ 0 & 1_s & 0 & 0 \\ 0 & 0 & T_{pg} & 0 \\ 0 & 0 & T_{tg} & 0 \end{bmatrix}$$

where $I_y = j_\phi^{(n-1)}(r_y, z_y) \Delta r \Delta z$; $T_{pg} = \sum_y T_{yg}$; and 1_a is the identity matrix. J_a and J_s are additional free parameters corresponding to uncertainties on coil currents measurements and vessel currents observer.

Introduction of weights This system is solved in a least square sense, each equation being given a weight $w...$ inversely proportional to the associated measurement error. In order to improve the algorithm, the block structure of the matrix is used:

$$Y_r = \begin{bmatrix} w_f \psi_f \\ w_m B_m \end{bmatrix} \quad Y_i = \begin{bmatrix} w_p I_p \\ w_t \Phi_t \end{bmatrix} \quad Y_e = \begin{bmatrix} w_a I_a \\ w_s I_s \end{bmatrix}$$

$$J_e = \begin{bmatrix} J_a \\ J_s \end{bmatrix} \quad a_j = \begin{bmatrix} a_g \\ \delta z \end{bmatrix}$$

which gives a more compact expression (weighted version of equation 6). \mathbf{AdG}_w is also the weighted expression of \mathbf{AdG} . This rewriting exhibits the linear regression at the core of the algorithm:

$$\begin{bmatrix} Y_r \\ Y_e \\ Y_i \end{bmatrix} = \mathbf{AdG}_w \cdot \begin{bmatrix} a_g \\ J_e \\ \delta z \end{bmatrix}$$

or, written more simply:

$$\mathbf{Y} = \mathbf{AdG}_w \cdot \mathbf{a}_G \quad (7)$$

The aim of the study is to analyse the influence of the weights choice on the regression, and the better value that should be applied to it.

1.2 Error propagation analysis

As the measurements made on the TCV coils have uncertainties, and as the LIUQE algorithm makes iterations on those measurements, it is necessary to study the error propagation.

In that purpose, the most common formula for the uncertainty of a variable R depending on N parameters x_i is the following differential :

$$\Delta R(x_1, \dots, x_N) = \left| \frac{\partial R}{\partial x_1} \right| \Delta x_1 + \dots + \left| \frac{\partial R}{\partial x_N} \right| \Delta x_N$$

where the Δ symbol denotes an uncertainty.

Nevertheless, this expression is incomplete as it is only of order 1, and it does not take in account the correlations between the parameters. These correlations could increase or decrease the global uncertainty of the variable R . Fortunately it is very easy to express thanks to a correlation matrix (cf annexes). In that way, the uncertainty formula can be rewritten at order 2 in terms of variance and covariance (cf [4], page 10):

$$\sigma_R^2 = (\nabla R)^T \cdot \widehat{\text{correl}}(\hat{\beta}) \cdot \nabla R \quad (8)$$

$$\sigma_R^2 = \sum_{i=1}^N \left| \frac{\partial R}{\partial x_i} \right|^2 \widehat{\text{correl}}(\hat{\beta})_{ii} + \underbrace{\sum_{i,j=1}^N \left| \frac{\partial R}{\partial x_i} \cdot \frac{\partial R}{\partial x_j} \right| \widehat{\text{correl}}(\hat{\beta})_{ij}}_{\text{off-diagonal terms}}$$

As the correlation matrix is symmetric, this last expression can be simplified by summing only on the upper side off to the diagonal :

$$\sigma_R^2 = \sum_{i=1}^N \left| \frac{\partial R}{\partial x_i} \right|^2 \widehat{\text{correl}}(\hat{\beta})_{ii} + 2 \underbrace{\sum_{i=1}^{N-1} \sum_{j=2}^N \left| \frac{\partial R}{\partial x_i} \cdot \frac{\partial R}{\partial x_j} \right| \widehat{\text{correl}}(\hat{\beta})_{ij}}_{\text{correlation terms}} \quad (9)$$

The off-diagonal terms are those related to correlations between parameters.

The exact formula for uncertainties is then:

$$\Delta R = \sqrt{\sigma_R^2} \quad (10)$$

2 Derivation of error propagations

2.1 Expression of the diagnostic functions

The two diagnostics from the TCV probes gives measurements of j_ϕ and p in the Grad-Shafranov equation (cf annex A.5). Therefore the error propagation study should begin from these quantities.

In LIUQE algorithm, the parametrization of the core equation 3 is linear :

$$j_\phi = \sum_g a_g r^{\nu_g} g_g(\psi(r, z + \delta z)) \quad (11)$$

with the notations :

$$\nu_1 = +1 \quad g_1 = (\psi - \psi_0) \quad \text{for } p' \quad (12)$$

$$\nu_2 = -1 \quad g_2 = (\psi - \psi_0) \quad \text{for } TT' \quad (13)$$

$$\nu_3 = -1 \quad g_3 = (\psi - \psi_0)(\psi - \psi_A) \quad \text{for } TT' \quad (14)$$

where ψ_0 is the flux function value at the border of the plasma, ψ_A is the value on the magnetic axis. The third linear function 14 comes only if the chosen model uses three basis functions.

The expression of the derivative function p' is then trivial (with a $2\pi r$ correction):

$$p'(\psi) = a_1 \cdot r^{+1} \frac{(\psi - \psi_0)}{2\pi r} = a_1 \frac{(\psi - \psi_0)}{2\pi}$$

Consequently, in this parametrization, the pressure p has the following expression (using the border condition $p = 0$ at $\psi = \psi_0$):

$$p(\psi) = \int_{\psi_0}^{\psi} p'(\phi) d\phi = \frac{a_1}{2\pi} \left(\frac{\psi^2}{2} - \psi\psi_0 + \frac{\psi_0^2}{2} \right) \quad (15)$$

For j_ϕ it is also obvious :

$$j_\phi(\psi) = a_1 \frac{(\psi - \psi_0)}{2\pi} + a_2 \frac{(\psi - \psi_0)}{r} + \underbrace{a_3 \frac{(\psi - \psi_0)(\psi - \psi_A)}{r}}_{\text{only with 3 basis functions}} \quad (16)$$

2.2 Related variance

Applying equation 9 for j_ϕ and p with respect to the parameters of the LIUQE regression gives the variances of the error propagation.

The derivatives are:

$$\begin{aligned} \frac{\partial j_\phi}{\partial a_1} &= \frac{(\psi - \psi_0)}{2\pi} \\ \frac{\partial j_\phi}{\partial a_2} &= \frac{(\psi - \psi_0)}{r} \\ \frac{\partial j_\phi}{\partial a_3} &= \frac{(\psi - \psi_0)(\psi - \psi_A)}{r} \\ \frac{\partial p}{\partial a_1} &= \frac{1}{2\pi} \left(\frac{\psi^2}{2} - \psi\psi_0 + \frac{\psi_0^2}{2} \right) \\ \frac{\partial p}{\partial a_2} &= 0 \\ \frac{\partial p}{\partial a_3} &= 0 \end{aligned}$$

and the variances are:

$$\begin{aligned} \sigma_{j_\phi}^2 &= \left(\frac{(\psi - \psi_0)}{2\pi} \right)^2 \widehat{\text{covar}}(\hat{\beta})_{57,57} \\ &+ \left(\frac{(\psi - \psi_0)}{r} \right)^2 \widehat{\text{covar}}(\hat{\beta})_{58,58} \\ &+ \left(\frac{(\psi - \psi_0)(\psi - \psi_A)}{r} \right)^2 \widehat{\text{covar}}(\hat{\beta})_{59,59} \\ &+ 2 \left| \frac{(\psi - \psi_0)}{2\pi} \frac{(\psi - \psi_0)}{r} \right| \widehat{\text{covar}}(\hat{\beta})_{57,58} \\ &+ 2 \left| \frac{(\psi - \psi_0)}{2\pi} \frac{(\psi - \psi_0)(\psi - \psi_A)}{r} \right| \widehat{\text{covar}}(\hat{\beta})_{57,59} \\ &+ 2 \left| \frac{(\psi - \psi_0)}{r} \frac{(\psi - \psi_0)(\psi - \psi_A)}{r} \right| \widehat{\text{covar}}(\hat{\beta})_{58,59} \quad (17) \end{aligned}$$

$$\sigma_p^2 = \left(\frac{1}{2\pi} \left(\frac{\psi^2}{2} - \psi\psi_0 + \frac{\psi_0^2}{2} \right) \right)^2 \widehat{\text{covar}}(\hat{\beta})_{57,57} \quad (18)$$

Taking the square root of these variances finally gives the errors.

3 Results and discussion

The LIUQE algorithm has been used during the whole study exclusively on the TCV shot n° 43760, at a time of 1 second.

3.1 Weights for plasma current I_p and toroidal flux Φ_t

The weights for plasma current I_p and toroidal flux Φ_t are first chosen for the study as they are related to the two diagnostic quantities in the Grad-Shafranov equation : j_ϕ and p' . w_t influences mainly p , as j_ϕ is influenced by both w_t and w_p . Consequently the fine tuning of those weights should have the stronger influence from all weights on the algorithm regression, and that is the reason why the study is focused on it.

The default values used in the LIUQE algorithm for w_p and w_t are:

$$w_p = (2400\text{A})^{-1} = 4.1667 \cdot 10^{-4} \text{A}^{-1}$$

$$w_t = (1.27 \cdot 10^{-4} \text{Wb})^{-1} = 7874 \text{Wb}^{-1}$$

The first part of the study consist into a research of minimal values of χ_{min}^2 , covariances and variances in the 2-D space of weights $\{w_t; w_p\}$, using a meshgrid. Preliminary results of the meshgrid with 2 basis functions are presented in figures 1a, 1b, and 1c. The first conclusion is that the variations of the studied quantities (minimal residual and variances) with respect to w_p are much weaker than along the w_t axis (a precise evaluation shows that it is of more than 8 orders of magnitude), and therefore not visible in this 3-D representation. Consequently, the two weights will be studied one after another.

3.1.1 Influence of w_t

Therefore, the influence of w_t is studied at a fixed value of 10^{-4}A^{-1} for w_p . Results are shown on figures 2, 3 and 4.

At fixed w_p , it appears that the covariance between parameters a_1 and a_2 tends towards zero when w_t increases. This means that the higher the w_t , the lower the correlations between these parameters.

3.1.2 Influence of w_p

As said before, the influence of w_p is extremely weak compared to the one of w_t . Results are shown on figures 5, 6 and 7.

Those graphs suggest that w_t should be increased in order to reduce the variance of parameters, and also the

correlation with the w_t parameter. Nevertheless, as it has a very weak influence, the improvement of the algorithm regression shall focus on the other parameters, especially w_t .

3.2 Error propagation

The values of pressure and current from the magnetic axis to the vessel are computed thanks to expressions 15, 16, and the equations of the subsection 2.2. The results given with LIUQE algorithm on the TCV shot #43760 are gathered in figure 8, for the two and three basis function models.

The model with two basis functions provides good results, as the standard error is 3.26% for the pressure and less than 2.10% for the current. At the opposite, the model with three basis functions is not trustworthy as the standard error is at 11.51% for pressure, and reaches values around 70% for current at some point of the axis. Note that the standard error for pressure does not depend on the radius as it is computed thanks to the square root of equation 18.

3.3 Discussion

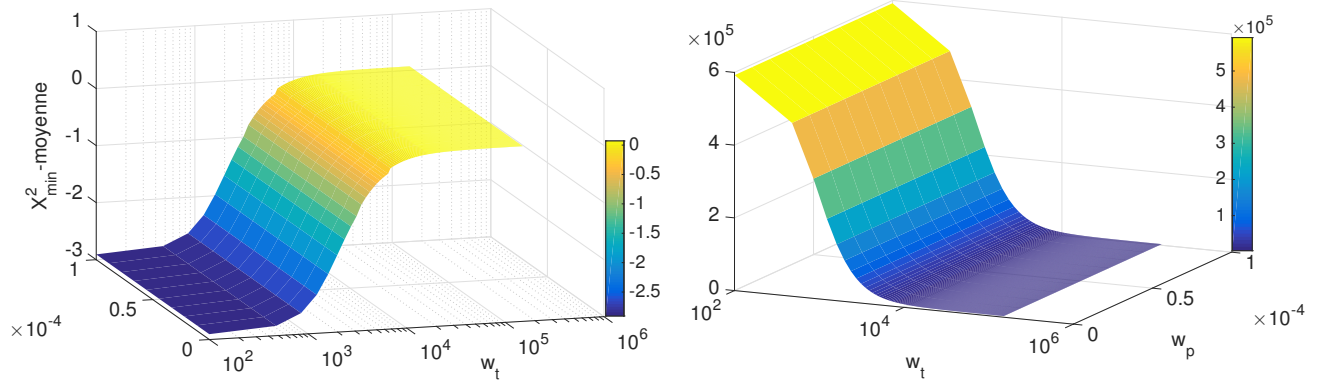
The weight study exhibits the importance of w_t : it should be increased in order to reduce the correlations with w_p . This study should also be systematized to the other weights in order to determine the overall parameters correlations.

The weak influence of w_p is not surprising at the end, as it is attached to the I_p plasma current calculation, which depends on the integration of magnetic field on the contour (cf [1], page 13):

$$I_p = I_{pm} \cdot B_m$$

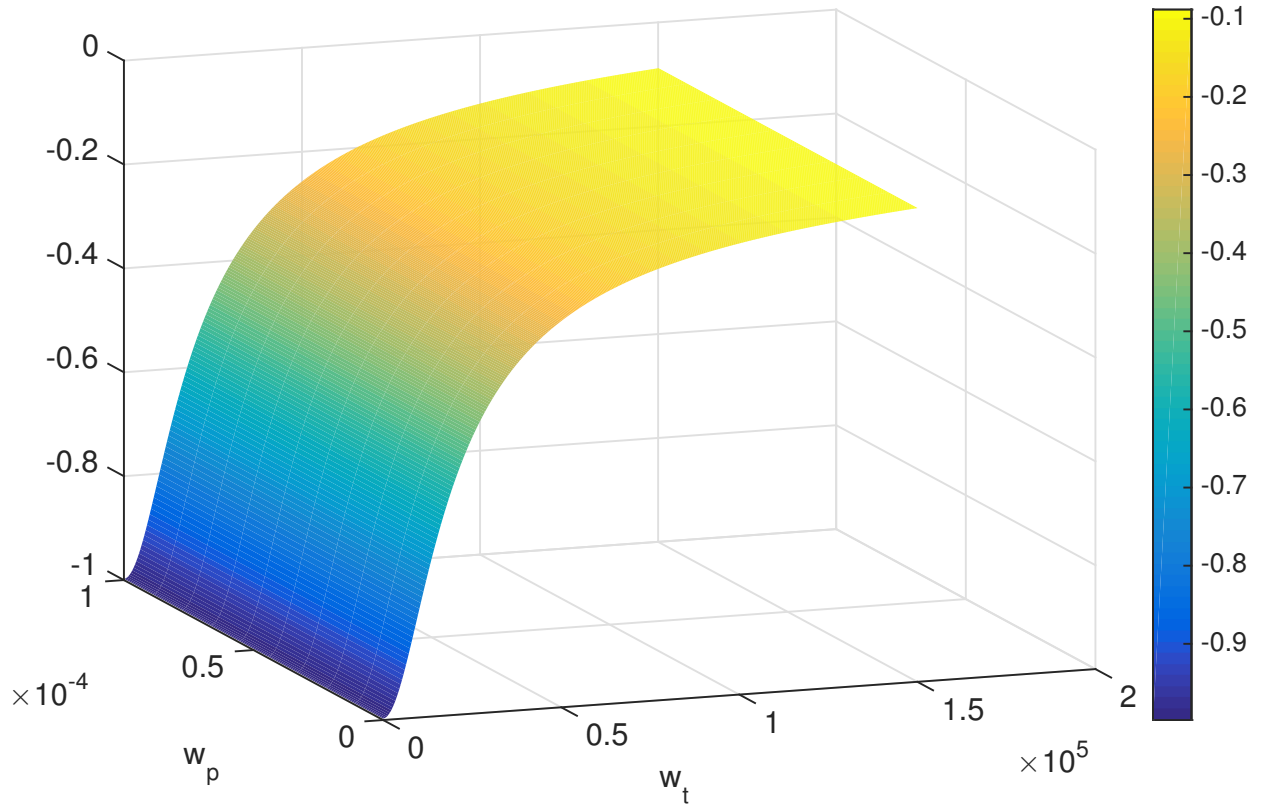
The B_m fields are already weighted with w_m . As the plasma current computation takes information on all of these fields, its weighting seems redundant. The algorithm is quite too general in the case of TCV as this equation is implicit, but it is a strength for adaptability for other tokamaks.

Finally, the study of error propagation confirms that the two basis function model is the most relevant for the LIUQE algorithm, as noted in the previous report.



(a) Surface of the minimal residual on a grid with weights w_t and w_p , plotted with the `surf` Matlab function. The w_t axis is logarithmic. The mean minimal residual value has been subtracted from the values in order to exhibit the variations around this mean value.

(b) Surface of the variance of parameter a_1 (from the correlation matrix) on a grid with weights w_t and w_p , plotted with the `surf` Matlab function. The w_t axis is logarithmic.



(c) Surface of the covariance between parameters a_1 and a_2 (from the covariance matrix) on a grid with weights w_t and w_p , plotted with the `surf` Matlab function. This covariance describe the correlation between the two parameters.

Figure 1: Graphs for the first 3D overview on the weights meshgrid.

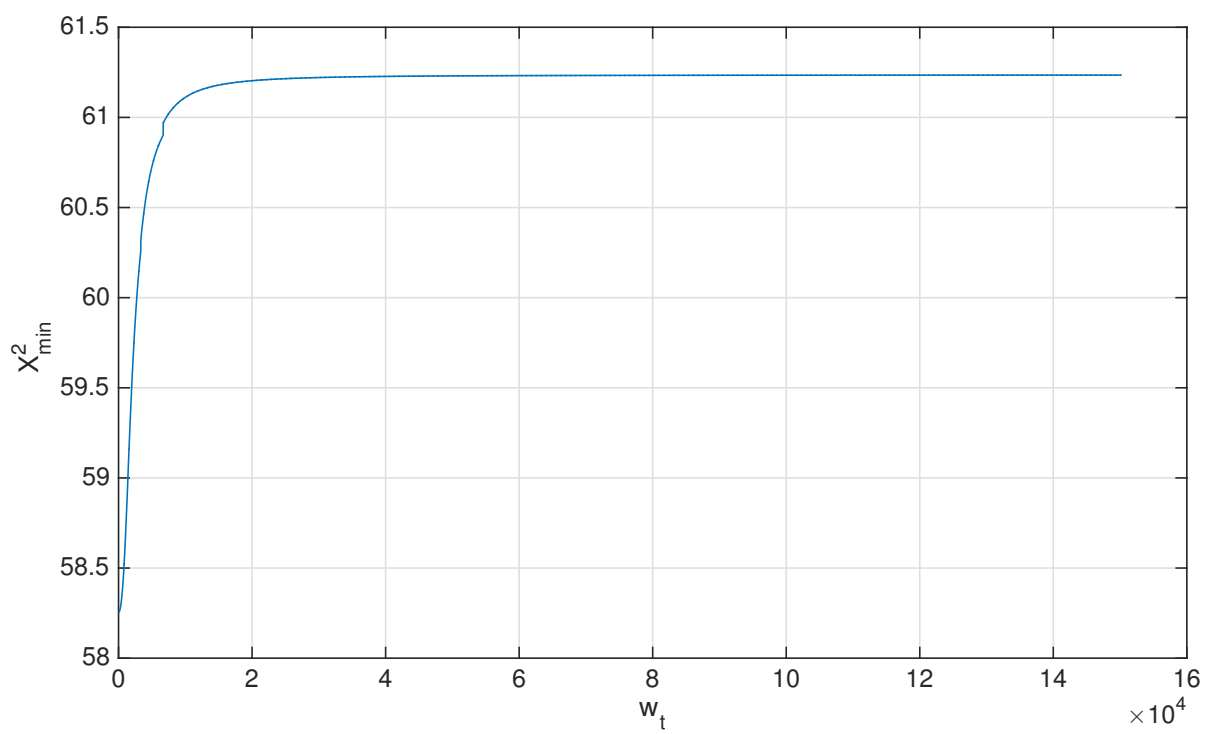


Figure 2: *Minimal residual versus weight w_t , at $w_p = 10^{-4} \text{A}^{-1}$.*

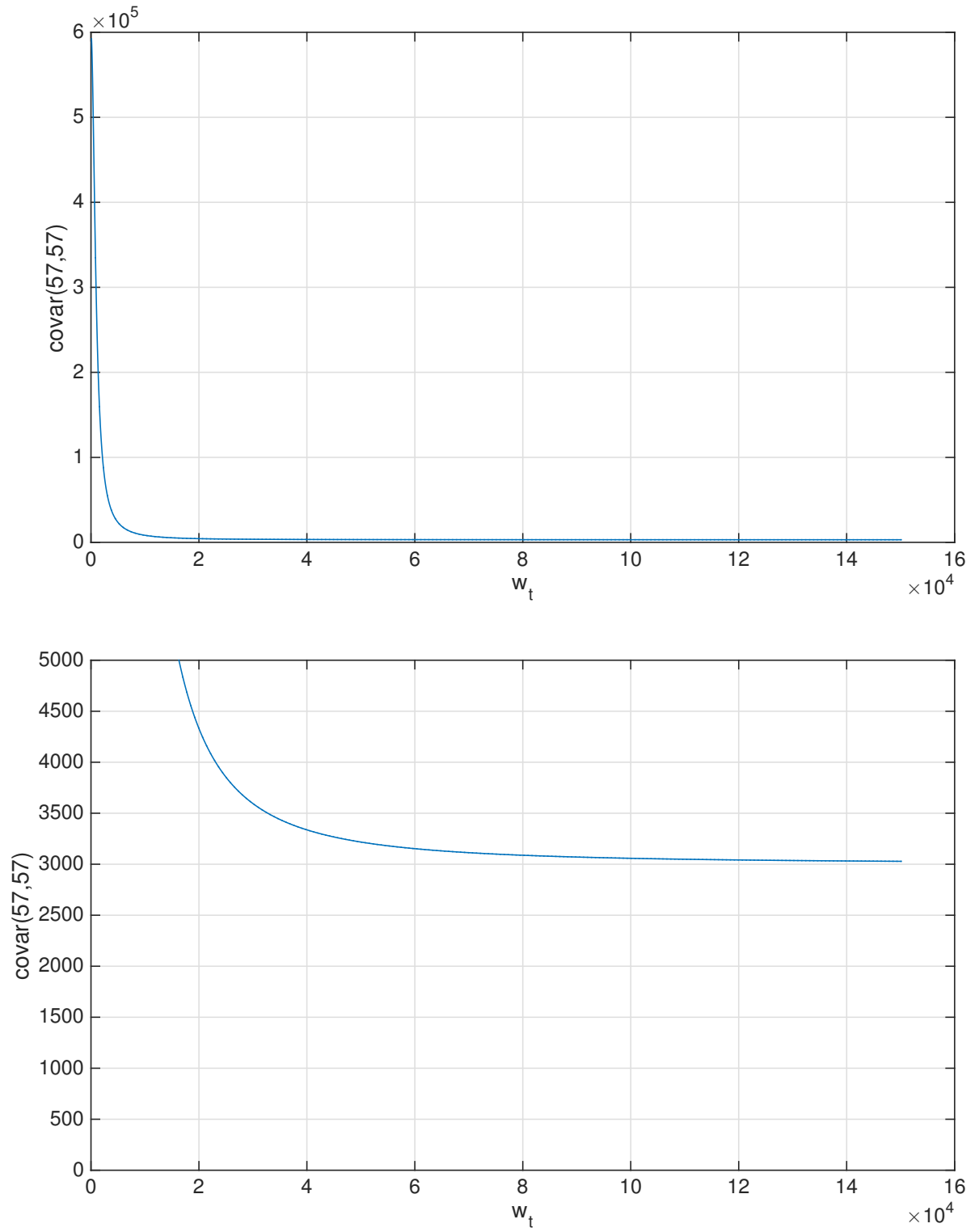


Figure 3: Variance of the parameter a_1 versus weight w_t , at $w_p = 10^{-4} \text{A}^{-1}$. A zoom in y -coordinates is applied for the second graph.

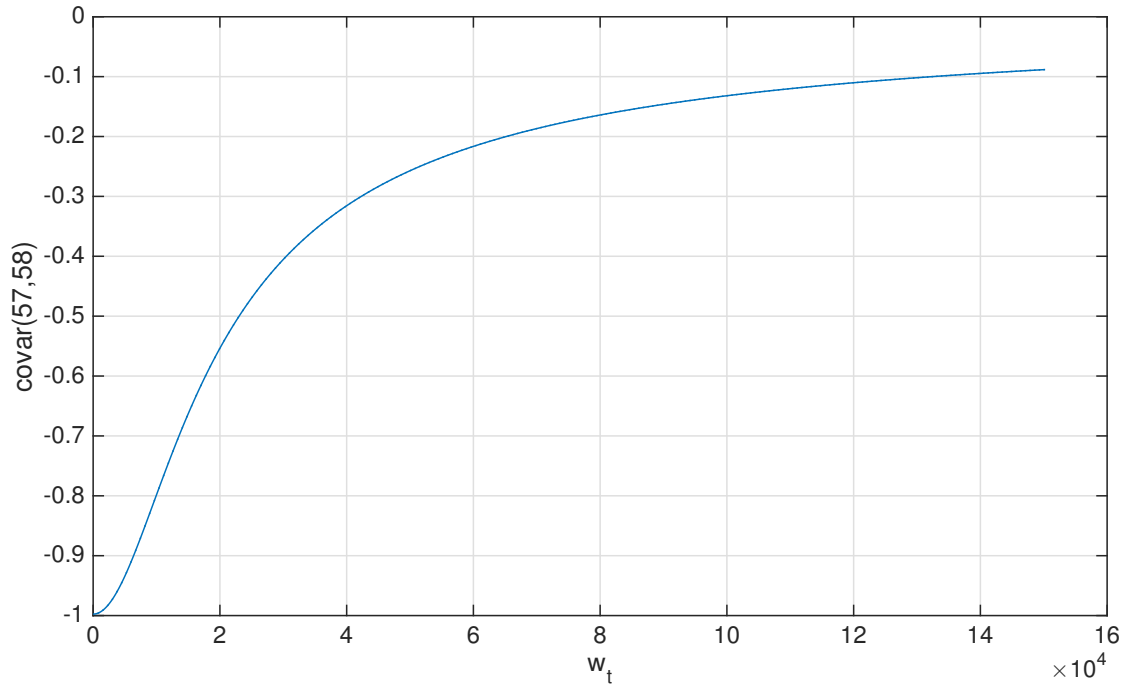


Figure 4: Normalized covariance between parameters a_1 and a_2 versus weight w_t , at $w_p = 10^{-4} \text{A}^{-1}$

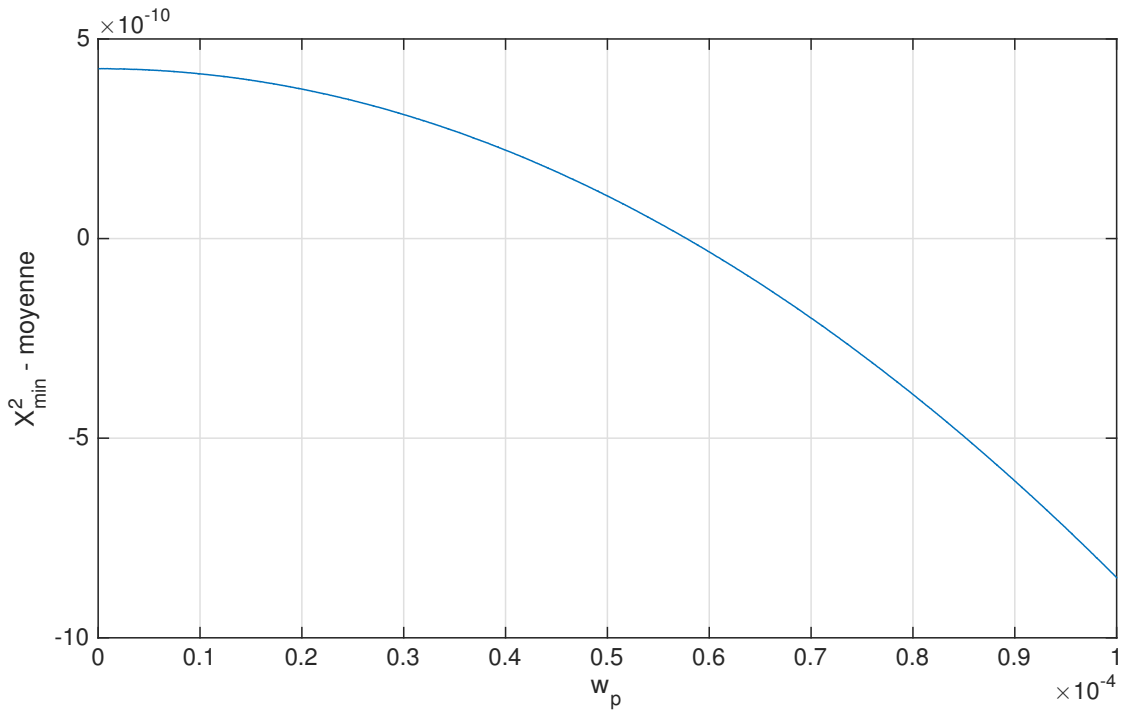


Figure 5: Minimal residual versus weight w_p , at $w_t = 8000 \text{Wb}^{-1}$. The mean value of the minimal residual, 61.0450, has been subtracted from the values in order to exhibit the variations around this mean value.

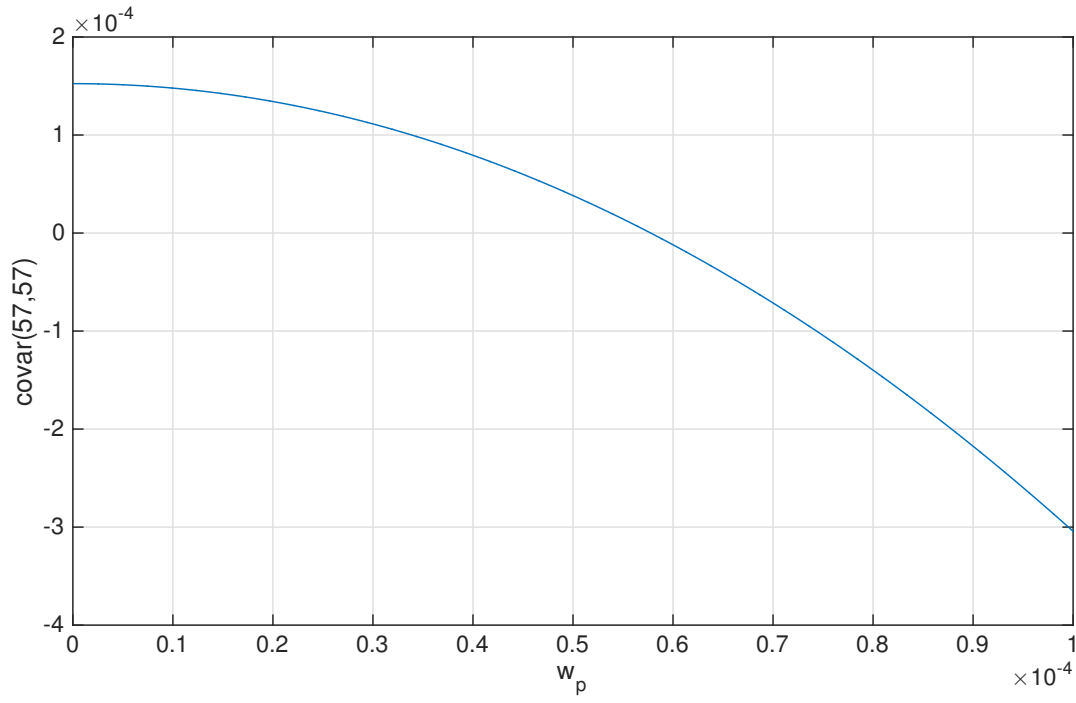


Figure 6: Variance of the parameter a_1 versus weight w_p , at $w_t = 8000\text{Wb}^{-1}$. The mean value of the variance, $1.1185 \cdot 10^4$, has been subtracted from the values in order to exhibit the variations around this mean value.

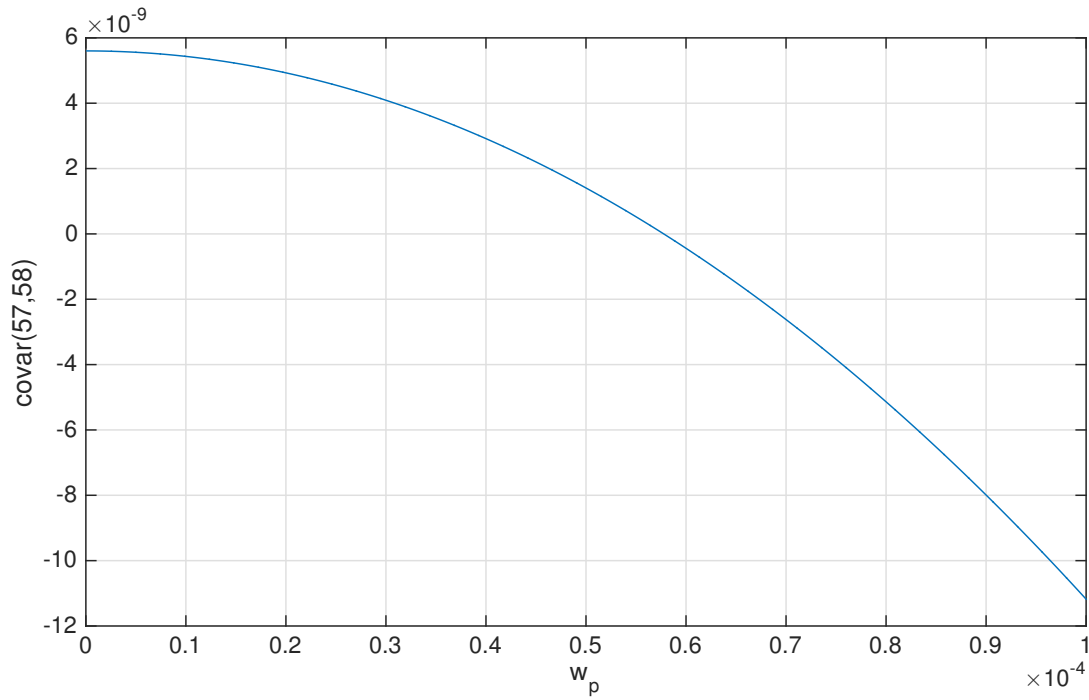
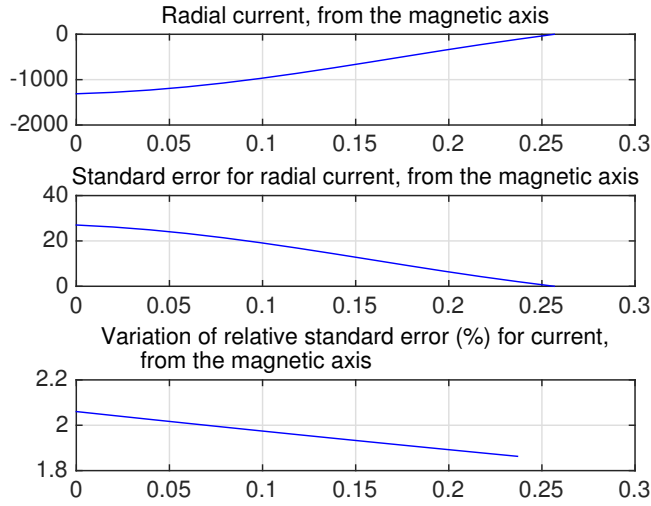
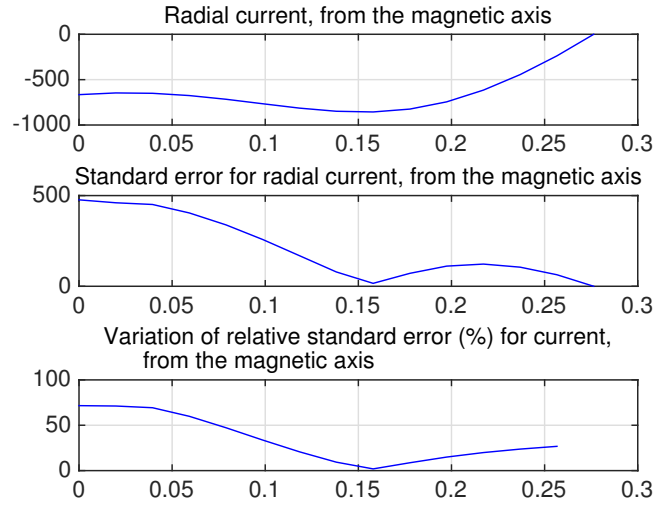


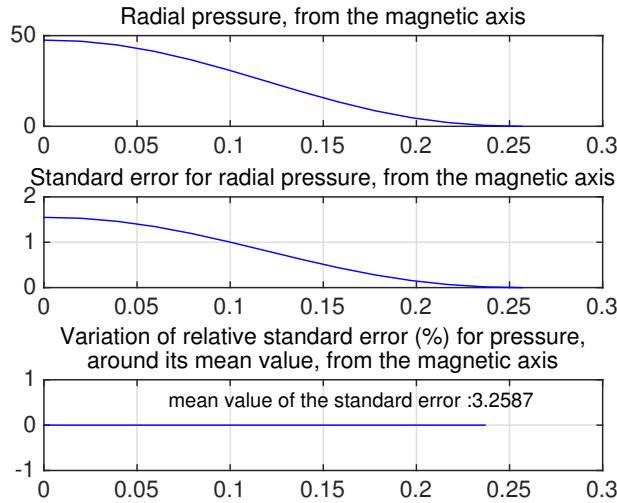
Figure 7: Covariance between parameters a_1 and a_2 versus weight w_p , at $w_t = 8000\text{Wb}^{-1}$. The mean value of the variance, -0.8556 , has been subtracted from the values in order to exhibit the variations around this mean value.



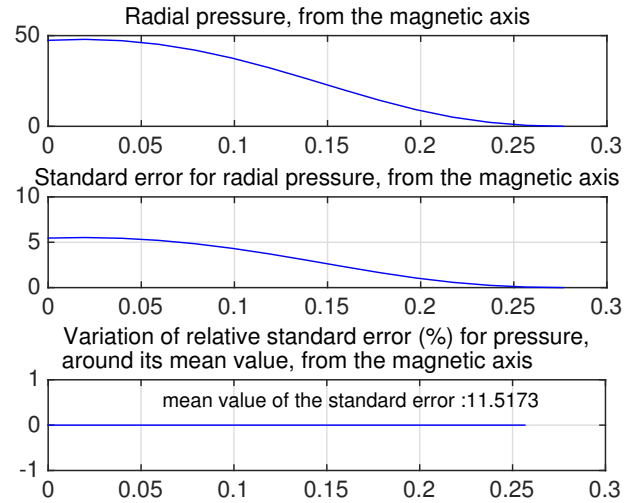
(a) Error propagation for the current, with the 2 basis function model.



(b) Error propagation for the current, with the 3 basis function model.



(c) Error propagation for the pressure, with the 2 basis function model. The mean value of standard error has been subtracted from the third graph in order to exhibit its constancy.



(d) Error propagation for the pressure, with the 3 basis function model. The mean value of standard error has been subtracted from the third graph in order to exhibit its constancy.

Figure 8: Graphs for error propagation study.

4 Possible directions for further improvement and research

As the correlations between w_t and other weights than w_p have not been treated, the study of the other weights in order to find the most impacting correlations would give the better choice of weights set in order to reduce the unuseful correlations between the parameters.

The analysis of the algorithm regression could also be applied on several other TCV shots, in order to verify the validity of the two basis function choice.

The propagation of errors from the current measurements to the basis function coefficient could also be studied more precisely.

Until now, the LIUQE algorithm applied on TCV has been proved to be very general and adaptable, so it should be very reliable on other tokamaks. The validity of the considerations on weights and error propagation on TCV should be conserved when applied on these other tokamaks, as the core of the LIUQE algorithm (e.g. Grad-Shafranov equation) remains.

References

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- [2] Miyamoto, *Plasma Physics for Nuclear Fusion*.
- [3] Sanford Weisberg, *Applied Linear Regression*.
- [4] J.Cartier, *Calcul de Sensibilités et prise en compte des Incertitudes sur les données dans les calculs d'Activation*, Réunion Incertitudes et Simulation - CEA/DIF - Jeudi 4 Octobre 2007.

A Annexes

A.1 Basics of linear regression

Linear regression analysis is a collection of methods whose aim is understanding relations between variables, in a quite simple and very elegant way. The simple regression assumes that two random variables (r.v.) Y and X are linearly connected together with the relationship:

$$Y = \beta_0 + \beta_1 X \quad (19)$$

where β_0 and β_1 are the exact coefficients of the linear equation. One need to add statistical error which can arise from several sources:

$$Y = \beta_0 + \beta_1 X + e \quad (20)$$

For the i -th measurement, the r.v. will take the experimental values y_i , x_i , and e_i :

$$y_i = \beta_0 + \beta_1 x_i + e_i \quad (21)$$

The equation 20 is supposed to represent the *real* physical correlation between Y and X , but it is obviously false. Therefore, the main aim of the experimental data treatment is to estimate the β_j coefficients from a set of measurements, obtaining a simple regression model:

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{e} \quad (22)$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are the estimates of β_0 and β_1 , and \hat{e} is called the residual. The "hat" notation will be used in the following to specify when a mathematical object is an estimate. The method focuses on finding the best estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ minimizing the so called *residual sum of squares* on the whole set of n measurements:

$$RSS(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2 = \sum_{i=1}^n e_i^2 \quad (23)$$

In the LIUQE case, the regression model has no constant β_0 coefficient, and is extended to multiple variables (p parameters, or r.v.). It still remains linear with respect to all of this new variables:

$$Y = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \dots + e \quad (24)$$

$$\hat{Y} = \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \hat{\beta}_3 X_3 + \dots + \hat{e} \quad (25)$$

These equations are commonly expressed in matrix notation for n measurements and p parameters:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e} \quad (26)$$

with the vectors and matrix:

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{e} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} \quad (27)$$

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \dots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix} \quad (28)$$

All vectors are written with bold symbols whereas scalar values are written normally. One has to be aware that \mathbf{X} is a $n * p$ -matrix and $\boldsymbol{\beta}$ a p -vector, whereas \mathbf{Y} and \mathbf{e} are n -vectors. This notation is very useful for simplification of calculus.

A.2 Minimization of the residual and variance ellipsoids

The residual of a multiple linear regression can be computed in matrix notation:

$$RSS(\boldsymbol{\beta}) = \sum_{i=1}^n (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2 = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) \quad (29)$$

For simplicity the residual will be denoted by $\chi^2 := RSS(\boldsymbol{\beta})$.

The estimate of the vector of regression coefficients is expressed by:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{Y}) \quad (30)$$

This estimate is the vector that minimizes the residual. Another useful expression is easily derivable from the last two result, isolating the minimal value of χ^2 :

$$\chi^2 = \chi_{min}^2 + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T (\mathbf{X}^T \mathbf{X}) (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \quad (31)$$

with

$$\chi_{min}^2 = (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \quad (32)$$

The second term on the right of equation 31 correspond to the parametrization of an ellipsoid centered on the point of coordinates $\hat{\boldsymbol{\beta}}$, in the space of coefficients $\{\beta_i\}$ of dimension p . In order to exhibit the equation of an ellipsoid, a *singular value decomposition* can be applied, leading to a diagonalisation of the $\mathbf{X}^T \mathbf{X}$ matrix:

$$\chi^2 = \chi_{min}^2 + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^T (\mathbf{U}^T \mathbf{S} \mathbf{U}) (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \quad (33)$$

\mathbf{S} is the diagonal matrix and \mathbf{U} is a unitary matrix. This equation can be understood with the following: the columns of \mathbf{U} give the axes of the ellipsoid in the coefficient space. Those vectors (noted \mathbf{U}_i for the i -th column) constitutes an orthonormal basis as \mathbf{U} is unitary. The eigenvalues on the diagonal of \mathbf{S} give the length of the semi-axes of the ellipsoid.

A.3 Variance and correlations

In matrix notation, the correlation matrix for the $\hat{\beta}_i$ parameters can be expressed as follows:

$$\text{correl}(\hat{\beta}) = \sigma^2(\mathbf{X}^T \mathbf{X})^{-1}$$

and its estimation:

$$\widehat{\text{correl}}(\hat{\beta}) = \hat{\sigma}^2(\mathbf{X}^T \mathbf{X})^{-1} \quad (34)$$

with the global estimator of variance (where p is the number of parameters in the model):

$$\hat{\sigma}^2 = \frac{\chi_{min}^2}{n - p} \quad (35)$$

This correlation matrix is normalizable in a *covariance matrix* in order to show clearly the correlations between parameters, avoiding the problem of different dimensions and order of magnitude. The normalization consists into dividing a correlation term between two parameters by the corresponding diagonal variances:

$$\left(\widehat{\text{covar}}(\hat{\beta})\right)_{ij} := \frac{\left(\widehat{\text{correl}}(\hat{\beta})\right)_{ij}}{\sqrt{\left(\widehat{\text{correl}}(\hat{\beta})\right)_{ii} \cdot \left(\widehat{\text{correl}}(\hat{\beta})\right)_{jj}}} \quad (36)$$

A.4 Relationship between the covariance matrix and the ellipsoids

It is possible to show that the correlation matrix diagonal gives the exact same maximal values of standard error as the projection of the standard error ellipsoid on the parameters axes, in the case $\chi = 2\chi_{min}^2$.

Noting that the points of the ellipsoid surface with maximal standard errors with regard to a parameter axis are those where the gradient is parallel to the parameter axis, one obtains:

$$\nabla \chi^2 = 2h_i \hat{\mathbf{e}}_i \quad (37)$$

where $\hat{\mathbf{e}}_i$ is the unit vector of the parameter axis and $2h_i$ is an arbitrary coefficient with convenient notation.

From equation 31 in the case $\chi = 2\chi_{min}^2$, the following comes:

$$\nabla \chi^2 = 2(\mathbf{X}^T \mathbf{X})(\beta - \hat{\beta}) \quad (38)$$

i.e. the vector $\beta - \hat{\beta}$ is known:

$$\beta - \hat{\beta} = h_i(\mathbf{X}^T \mathbf{X})^{-1} \hat{\mathbf{e}}_i \quad (39)$$

This vectors goes from the center of the ellipsoid at $\hat{\beta}$ to the point β where the gradient is null. Replacing it in equation 31, one gets:

$$\chi^2 = 2\chi_{min}^2 = \chi_{min}^2 + h_i^2 \hat{\mathbf{e}}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \hat{\mathbf{e}}_i$$

or, after the writing of the products with $\hat{\mathbf{e}}_i$ vectors:

$$\chi_{min}^2 = h_i^2 \sum_{kl} \delta_{ik} (\mathbf{X}^T \mathbf{X})_{kl}^{-1} \delta_{li} = h_i^2 (\mathbf{X}^T \mathbf{X})_{ii}^{-1}$$

So the coefficient has now the expression:

$$h_i = \frac{\chi_{min}}{\sqrt{(\mathbf{X}^T \mathbf{X})_{ii}^{-1}}} \quad (40)$$

The refreshment of equation 39 gives:

$$\beta - \hat{\beta} = \frac{\chi_{min}}{\sqrt{(\mathbf{X}^T \mathbf{X})_{ii}^{-1}}} (\mathbf{X}^T \mathbf{X})^{-1} \hat{\mathbf{e}}_i \quad (41)$$

In order to get the maximal standard error for the i -th parameter, one has to compute the corresponding component of equation 41. In the simplest case where $n - p = 1$, we get:

$$\begin{aligned} \beta_i - \hat{\beta}_i &= \frac{\chi_{min}}{\sqrt{(\mathbf{X}^T \mathbf{X})_{ii}^{-1}}} \sum_k (\mathbf{X}^T \mathbf{X})_{ik}^{-1} \delta_{ki} \\ &= \frac{\chi_{min}}{\sqrt{(\mathbf{X}^T \mathbf{X})_{ii}^{-1}}} (\mathbf{X}^T \mathbf{X})_{ii}^{-1} \\ &= \sqrt{(\mathbf{X}^T \mathbf{X})_{ii}^{-1}} \chi_{min} \\ &= \sqrt{\widehat{\text{correl}}(\hat{\beta})_{ii}} \end{aligned}$$

Consequently, when $\chi = 2\chi_{min}^2$, the correlation matrix diagonal gives the exact same maximal values of standard error as the projection of the standard error ellipsoid on the parameters axes.

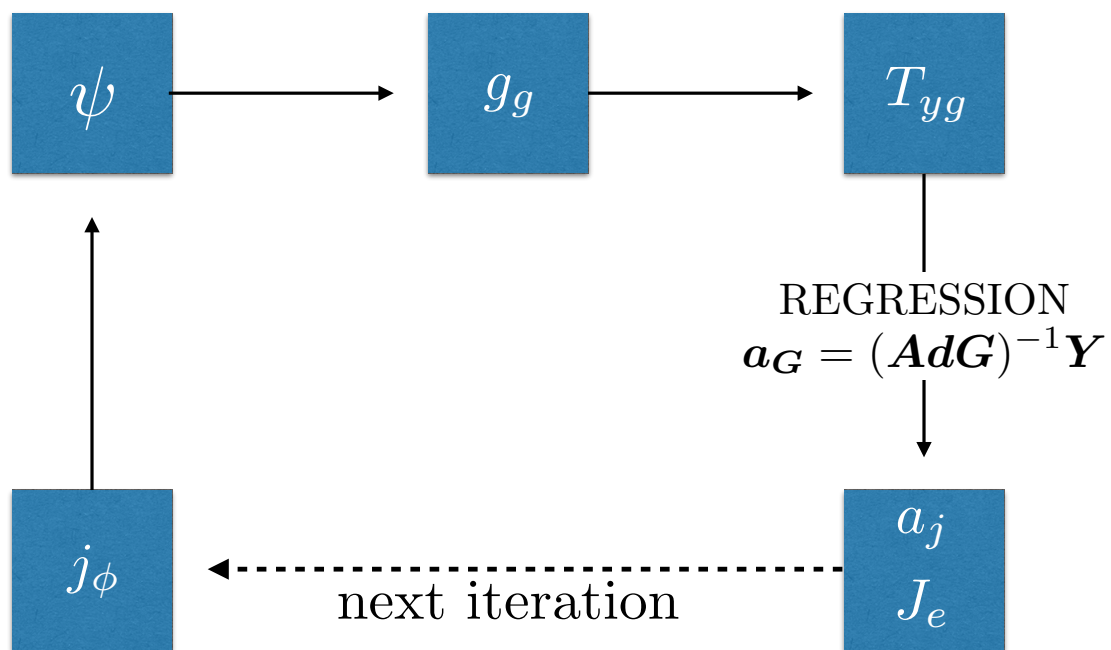
A.5 LIUQE regression loop

LIUQE algorithm relies on this single linear regression:

$$\mathbf{a}_G = (\mathbf{AdG})^{-1} \mathbf{Y} \quad (42)$$

All the equations from the previous subsection about linear regression analysis are then applicable with $\mathbf{AdG} := \mathbf{X}$ and $\mathbf{a}_G := \beta$.

The complete algorithm loop is summarized on figure 9.

Figure 9: *LIUQE algorithm loop.*